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INTRODUCTION TO NUMERICAL EVALUATION OF COMPARATIVE MODELS

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Measures applied in the evaluation of Comparative Models are presented. These include RMS deviation in atomic positions and dihedral angles as well as deviation in error estimates. Several exclusions are employed to filter out the influence of possible experimental uncertainties: thermal motion, disorder, intermolecular contacts in the crystal, and atomic assignment deemed unreliable crystallographically. A number of subsets select for regions of structure difficult to model. These subsets allow to focus on sidechains which are rotamerically different in the parent structure, structure segments shifted relative to parent, favorable alternative parent selections, and loops. The last group of subsets specifies surface and core regions, as well as regions of structure in contact with ligand(s).

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